

On Three Imaginary-time Path Integral Formulas with Magnetic Fields in Relativistic Quantum Mechanics *

By

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Abstract

Three magnetic relativistic Schrödinger operators are considered, corresponding to the classical relativistic Hamiltonian symbol with both magnetic vector and electric scalar potentials. Path integral representations for the solutions of their respective imaginary-time relativistic Schrödinger equations, i.e. heat equations are given in two ways. The one is by means of the probability path space measure coming from the Lévy process concerned, and the other is through time-sliced approximation with Chernoff's theorem.

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References

§ 1. Introduction

Path integral is a marvelous idea invented by R. P. Feynman ([F-48], [F-05], [FH-65]. cf. [D-33,35], [D-45]) to give a practically very useful and now figurative sublimed way to write down the solution of the *real-time* Schrödinger equation in nonrelativistic quantum mechanics.

In this paper, we deal with the problem in relativistic quantum mechanics to consider the relativistic Schrödinger equation in *imaginary time*. In the literature there are 3 kinds of relativistic Schrödinger operators $H = H_A + V$ for a spinless particle of mass $m \geq 0$ corresponding to

$$(1.1) \quad \sqrt{(\xi - A(x))^2 + m^2} + V(x), \quad (\xi, x) \in \mathbf{R}^d \times \mathbf{R}^d,$$

under magnetic vector potential $A(x)$ and electric scalar potential $V(x)$, depending on *how to quantize the kinetic energy term* $\sqrt{(\xi - A(x))^2 + m^2}$. This H is used in the situation where we may ignore QFT effect like particles creation and annihilation, but should take relativistic effect into consideration.

We give three path integral representation formulas for the solutions for their respective imaginary-time relativistic Schrödinger equations, i.e. heat equations, by means of the probability path space measure coming from Lévy process concerned. We also discuss the path integral by time-sliced approximation. It is well-known that this method also can plainly give a meaning for Schrödinger equation by the Trotter–Kato product formula, if the Schrödinger operator has only electric scalar potential. But if it has also *magnetic vector potential*, we should use Chernoff’s theorem instead. This wisdom also applies to Dirac equation.

This paper is of expository character, having in sections 2 and 3 description and content which overlap with another a little more elaborate paper on the subject in *RIMS Kyoto Univ. Kôkyûroku* **1797**(2012) [I-12a]. Their detailed version was in the meanwhile published in my paper [I-13] and also brief note [I-12b]. So I would not like to repeat the whole story here but only to write a short survey describing the points how to obtain the three path integral representation formulas with sketch of proof. In §4, the path integral by time-sliced approximation is further studied for some other evolution equations in quantum mechanics in real and imaginary time by means of *Chernoff’s theorem*, also discussing its convergence, not only in strong topology, but also in operator norm and pointwise for the integral kernels. The content is almost independent of the three relativistic Schrödinger operators up to the previous section. The observation of this last section might contain something new.

For the reader's convenience, the table of contents of [I-13] is as follows:

1. Introduction;
2. Three magnetic relativistic Schrödinger operators: 2.1.Their definition and difference; 2.2.Gauge-covariant or not;
3. More general definition of magnetic relativistic Schrödinger operators and their selfadjointness: 3.1.The most general definition of $H_A^{(1)}$, $H_A^{(2)}$ and $H_A^{(3)}$; 3.2.Selfadjointness with negative scalar potentials;
4. Imaginary-time path integrals for magnetic relativistic Schrödinger operators: 4.1.Feynman–Kac–Itô type formulas for magnetic relativistic Schrödinger operators; 4.2.Heuristic derivation of path integral formulas;
5. Summary

§ 2. Three magnetic relativistic Schrödinger operators

The three relativistic Schrödinger operators concerned are the following. The first one is the Weyl pseudo-differential operator defined through mid-point prescription $H^{(1)} := H_A^{(1)} + V$ considered by Ichinose and Tamura ([IT-86], [I-89, 95], [NaU-90]), the second $H^{(2)} := H_A^{(2)} + V$ the modification of the first one by Iftimie, Măntoiu and R. Purice [IfMP-07, 08, 10], and the third $H^{(3)} := H_A^{(3)} + V$ defined with the square root $H_A^{(3)}$ of the nonnegative selfadjoint operator $(-i\nabla - A(x))^2 + m^2$.

For simplicity, assume that $A(x)$ is smooth and $V(x)$ bounded below.

(1) Weyl pseudo-differential operator $H^{(1)} := H_A^{(1)} + V$ (e.g. [IT-86; I-89, 95]) with

$$(2.1) \quad \begin{aligned} (H_A^{(1)} f)(x) &:= \frac{1}{(2\pi)^d} \iint_{\mathbf{R}^d \times \mathbf{R}^d} e^{i(x-y) \cdot \xi} \sqrt{\left(\xi - A\left(\frac{x+y}{2}\right)\right)^2 + m^2} f(y) dy d\xi \\ &= \frac{1}{(2\pi)^d} \iint_{\mathbf{R}^d \times \mathbf{R}^d} e^{i(x-y) \cdot (\xi + A(\frac{x+y}{2}))} \sqrt{\xi^2 + m^2} f(y) dy d\xi. \end{aligned}$$

Here, with $f \in C_0^\infty(\mathbf{R}^d)$ or $f \in \mathcal{S}(\mathbf{R}^d)$, the integrals on the right-hand side are oscillatory integrals.

(2) Modified Weyl pseudo-differential operator $H^{(2)} := H_A^{(2)} + V$ [IfMP-07, 08, 10] with

$$(2.2) \quad \begin{aligned} (H_A^{(2)} f)(x) &:= \frac{1}{(2\pi)^d} \iint_{\mathbf{R}^d \times \mathbf{R}^d} e^{i(x-y) \cdot \xi} \sqrt{\left(\xi - \int_0^1 A((1-\theta)x + \theta y) d\theta\right)^2 + m^2} f(y) dy d\xi \\ &= \frac{1}{(2\pi)^d} \iint_{\mathbf{R}^d \times \mathbf{R}^d} e^{i(x-y) \cdot (\xi + \int_0^1 A((1-\theta)x + \theta y) d\theta)} \sqrt{\xi^2 + m^2} f(y) dy d\xi \end{aligned}$$

(3) $H^{(3)} := H_A^{(3)} + V$ defined with square root

$$(2.3) \quad H_A^{(3)} := \sqrt{(-i\nabla - A(x))^2 + m^2}$$

of the nonnegative selfadjoint operator $(-i\nabla - A(x))^2 + m^2$. This $H^{(3)}$ is used, e.g., to study “stability of matter” in relativistic quantum mechanics in Lieb–Seiringer [LSei-10].

Known facts for $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$

1°. With suitable reasonable conditions on $A(x)$ and $V(x) \geq 0$, they all define *selfadjoint* operators in $L^2(\mathbf{R}^d)$, which are bounded below. For instance, they become selfadjoint operators defined as quadratic forms, for $H^{(1)}$ and $H^{(2)}$, when $A \in L_{loc}^{1+\delta}(\mathbf{R}^d; \mathbf{C}^d)$ for some $\delta > 0$ and $V \in L_{loc}^1(\mathbf{R}^d)$ (cf. [I-89, 13], [IfMP-07, 08, 10]), while for $H^{(3)}$, when $A \in L_{loc}^2(\mathbf{R}^d; \mathbf{C}^d)$ and $V \in L_{loc}^1(\mathbf{R}^d)$ (e.g. [CFKS-87, pp.8–10] or [I-13]).

In fact further, they are bounded below by the *same lower bound*, in particular,

$$(2.4) \quad H_A^{(j)} \geq m, \quad j = 1, 2, 3.$$

2°. $H_A^{(2)}$ and $H_A^{(3)}$ are covariant under gauge transformation, i.e. it holds for every $\varphi \in \mathcal{S}(\mathbf{R}^d)$ that $H_{A+\nabla\varphi}^{(j)} = e^{i\varphi} H_A^{(j)} e^{-i\varphi}$, $j = 2, 3$. However, $H_A^{(1)}$ is not.

3°. All these three operators are different in general, but coincide, if $A(x)$ is linear in x , i.e. if $A(x) = \dot{A} \cdot x$ with $\dot{A} : d \times d$ real symmetric *constant matrix*, then $H_A^{(1)} = H_A^{(2)} = H_A^{(3)}$. So, this holds for uniform magnetic fields with $d = 3$.

§ 3. Imaginary-time Path integral for magnetic relativistic Schrödinger operators

For each $H = H_A + V$ of the three magnetic relativistic Schrödinger operators $H^{(1)} = H_A^{(1)} + V$, $H^{(2)} = H_A^{(2)} + V$ and $H^{(3)} = H_A^{(3)} + V$, consider imaginary-time relativistic Schrödinger equation

$$(3.1) \quad \begin{cases} \frac{\partial}{\partial t} u(t, x) = -[H - m]u(t, x), & t > 0, \\ u(0, x) = g(x), & x \in \mathbf{R}^d. \end{cases}$$

The solution of this Cauchy problem is given by the semigroup $u(t, x) = (e^{-t[H-m]}g)(x)$. We want to find a path integral formula for each $e^{-(H^{(j)}-m)}g$, $j = 1, 2, 3$.

§ 3.1. The case for the Weyl pseudo-differential operator $H^{(1)} = H_A^{(1)} + V$

$H_A^{(1)}$, in (2.1), can be rewritten as an integral operator:

$$(3.2) \quad \begin{aligned} ([H_A^{(1)} - m]f)(x) &= - \int_{|y|>0} [e^{-iy \cdot A(x + \frac{y}{2})} f(x+y) - f(x) \\ &\quad - I_{\{|y|<1\}} y \cdot (\nabla - iA(x)) f(x)] n(dy) \\ &= - \lim_{r \downarrow 0} \int_{|y| \geq r} [e^{-iy \cdot A(x + \frac{y}{2})} f(x+y) - f(x)] n(dy) \\ &= - \text{p.v.} \int_{|y|>0} [e^{-iy \cdot A(x + \frac{y}{2})} f(x+y) - f(x)] n(dy) \end{aligned}$$

where $n(dy) = n(y)dy$ is an m -dependent measure on $\mathbf{R}^d \setminus \{0\}$, called *Lévy measure*, with density

$$n(y) = \begin{cases} 2(2\pi)^{-(d+1)/2} m^{d+1} (m|y|)^{-(d+1)/2} K_{(d+1)/2}(m|y|), & m > 0, \\ \pi^{-(d+1)/2} \Gamma\left(\frac{d+1}{2}\right) |y|^{-(d+1)}, & m = 0 \end{cases}$$

It appears in the *Lévy–Khinchin formula* :

$$(3.3) \quad \sqrt{\xi^2 + m^2} - m = - \int_{|y|>0} (e^{iy \cdot \xi} - 1 - i\xi \cdot y I_{\{|y|<1\}}) n(dy) = - \lim_{r \rightarrow 0+} \int_{|z| \geq r} (e^{iz \cdot \xi} - 1) n(dz)$$

Proof of (3.2). By the Lévy–Khinchin formula (3.3),

$$\begin{aligned} (H_A^{(1)} f)(x) &= (2\pi)^{-d} \int \int e^{i(x-y) \cdot (\xi + A(\frac{x+y}{2}))} \left[m - \lim_{r \rightarrow 0+} \int_{|z| \geq r} (e^{iz \cdot \xi} - 1) n(dz) \right] f(y) dy d\xi \\ &= (2\pi)^{-d} \left[m \int \int e^{i(x-y) \cdot \xi} e^{i(x-y) \cdot A(\frac{x+y}{2})} dy d\xi \right. \\ &\quad \left. - \lim_{r \rightarrow 0+} \int \int \int_{|z| \geq r} (e^{i(x-y+z) \cdot \xi} - e^{i(x-y) \cdot \xi}) n(dz) e^{i(x-y) \cdot A(\frac{x+y}{2})} f(y) dy d\xi \right] \\ &= m \int \delta(x-y) e^{i(x-y) \cdot A(\frac{x+y}{2})} f(y) dy \\ &\quad - \lim_{r \rightarrow 0+} \int \int_{|z| \geq r} (\delta(x-y+z) - \delta(x-y)) n(dz) e^{i(x-y) \cdot A(\frac{x+y}{2})} f(y) dy \\ &= m f(x) - \lim_{r \rightarrow 0+} \int \int_{|z| \geq r} (e^{-iz \cdot A(x+\frac{z}{2})} f(x+z) - f(x)) n(dz) \end{aligned}$$

□

Some Notations from Lévy process to represent $e^{-t[H^{(1)}-m]}g$ by path integral

For more details, we refer to [IkW-81, 89].

$\cdot D_x([0, \infty) \rightarrow \mathbf{R}^d)$: space of right-continuous paths $X : [0, \infty) \rightarrow \mathbf{R}^d$ with left-hand limits (called “*càdlàg* paths”) with $X(0) = x$

$\cdot \lambda_x$: probability measure on $D_x([0, \infty) \rightarrow \mathbf{R}^d)$ such that

$$(3.4) \quad e^{-t[\sqrt{\xi^2 + m^2} - m]} = \int_{D_x([0, \infty) \rightarrow \mathbf{R}^d)} e^{i(X(t)-x) \cdot \xi} d\lambda_x(X), \quad t \geq 0, \xi \in \mathbf{R}^d$$

$\cdot N_X(dsd y)$: *counting measure* on $[0, \infty) \times (\mathbf{R}^d \setminus \{0\})$ to count the number of discontinuities of the path $X(\cdot)$, i.e. $N_X((t, t'] \times U) := \#\{s \in (t, t']; 0 \neq X(s) - X(s-) \in U\}$ ($0 < t < t', U \subset \mathbf{R}^d \setminus \{0\}$: Borel set). It satisfies $\int_{D_x} N_X(dsd y) d\lambda_x(X) = ds n(dy)$.

$\cdot \tilde{N}_X(dsd y) := N_X(dsd y) - ds n(dy)$

Then any path $X \in D_x([0, \infty) \rightarrow \mathbf{R}^d)$ can be expressed with $N_x(\cdot)$, $\tilde{N}_X(\cdot)$ as

$$X(t) = x + \int_0^{t+} \int_{|y| \geq 1} y N_X(ds dy) + \int_0^{t+} \int_{0 < |y| < 1} y \tilde{N}_X(ds dy).$$

Theorem 3.1. [ITa-86, I-95]

$$(3.5) \quad (e^{-t[H^{(1)}-m]}g)(x) = \int_{D_x([0, \infty) \rightarrow \mathbf{R}^d)} e^{-S^{(1)}(t, X)} g(X(t)) d\lambda_x(X),$$

$$S^{(1)}(t, X) = i \int_0^{t+} \int_{|y| \geq 1} A(X(s-) + \frac{y}{2}) \cdot y N_X(ds dy)$$

$$+ i \int_0^{t+} \int_{0 < |y| < 1} A(X(s-) + \frac{y}{2}) \cdot y \tilde{N}_X(ds dy)$$

$$+ i \int_0^t ds \text{ p.v. } \int_{0 < |y| < 1} A(X(s) + \frac{y}{2}) \cdot y n(dy) + \int_0^t V(X(s)) ds.$$

For some recent related result on the mass-zero limit problem with $H^{(1)}$, see [IM-14].

Proof (Sketch). Let $k_0(t, x - y)$ be the integral kernel of $e^{-t(\sqrt{-\Delta+m^2}-m)}$, put

$$(3.6) \quad (F(t)g)(x) := \int_{\mathbf{R}^d} k_0(t, x - y) e^{-iA(\frac{x+y}{2}) \cdot (y-x) - V(\frac{x+y}{2})t} g(y) dy,$$

which can be rewritten as

$$(3.7) \quad (F(t)g)(x) = \int_{D_x} e^{-iA(\frac{x+X(t)}{2}) \cdot (X(t)-x) - V(\frac{x+X(t)}{2})t} g(X(t)) d\lambda_x(X).$$

For the definition (3.6), note the second expression of the definition (2.1) of $H_A^{(1)}$.

Then we do partition of the time interval $[0, t]$ into n small subintervals with the same width t/n : $0 = t_0 < t_1 < \dots < t_n = t$, $t_j - t_{j-1} = t/n$, and put

$$(3.8) \quad S_n(x_0, \dots, x_n) := i \sum_{j=1}^n A\left(\frac{x_{j-1}+x_j}{2}\right) \cdot (x_j - x_{j-1}) + \sum_{j=1}^n V\left(\frac{x_{j-1}+x_j}{2}\right) \frac{t}{n},$$

$$x_j := X(t_j) (j = 0, 1, 2, \dots, n); x = x_0 := X(t_0), x_n := X(t_n) \equiv X(t),$$

where note that the assignment $t_j \mapsto X(t_j)$ is in the reversed time order.

Substitute these $n+1$ points of path $X(\cdot)$ into $S_n(x_0, \dots, x_n)$ to get

$$(3.9) \quad S_n(X) := S_n(X(t_0), \dots, X(t_n))$$

$$= i \sum_{j=1}^n A\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \cdot (X(t_j) - X(t_{j-1})) + \sum_{j=1}^n V\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \frac{t}{n}.$$

Then the n times product of $F(t/n)$ turns out

$$\begin{aligned}
 (F(t/n)^n g)(x) &= \overbrace{\int_{\mathbf{R}^d} \cdots \int_{\mathbf{R}^d}}^{n \text{ times}} \prod_{j=1}^n k_0(t/n, x_{j-1} - x_j) e^{-S_n(x_0, \dots, x_n)} g(x_n) dx_1 \cdots dx_n \\
 (3.10) \quad &= \int_{D_x} e^{-S_n(X)} g(X(t)) d\lambda_x(X) \\
 &= \int_{D_x} e^{-i \sum_{j=1}^n A\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \cdot (X(t_j)-X(t_{j-1})) - \sum_{j=1}^n V\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \frac{t}{n}} \\
 &\quad \times g(X(t)) d\lambda_x(X).
 \end{aligned}$$

We have to show convergence of each side of (3.10).

We shall use *Chernoff's theorem* for the left-hand side (LHS), while *Itô formula* for the right-hand side (RHS).

Proof of convergence of LHS of (3.10). We need

Lemma A. $F(t/n)^n g \rightarrow e^{-t[H^{(1)}-m]}g$ in $L^2(\mathbf{R}^d)$, $n \rightarrow \infty$.

The proof of Lemma A is essentially an application of the Chernoff's theorem, although it was proved directly in [ITa-86] or [I-13]. Note here that if the vector potential $A(x)$ is present, one cannot use the Trotter–Kato product formula instead of the Chernoff's theorem.

Chernoff's Theorem. [Ch-74] *Let F be a strongly continuous function on $[0, \infty)$ with values in the Banach space $\mathcal{L}(\mathbf{X})$ of bounded linear operators on a Banach space \mathbf{X} . Assume that F further satisfies the following conditions: (i) $F(0) = I$ (I : identity operator on \mathbf{X}), and there exists a real a such that $\|F(t)\| \leq e^{at}$ for all $t \geq 0$; (ii) The linear operator $F'(0) \upharpoonright_{D[F'(0)]}$ is closable, and the closure $\overline{F'(0)} := L$ generates a strongly continuous semigroup e^{-tL} .*

Then $F(t/n)^n$ converges to e^{-tL} strongly, as $n \rightarrow \infty$, uniformly on each finite interval in $t \geq 0$.

Note that condition (ii) means nothing but that $u(t) := e^{-tL}u_0$ is the solution of equation $\frac{d}{dt}u(t) = -Lu(t)$ with initial data $u(0) = u_0$. In §4, we shall give some observation on Chernoff's theorem as to how useful it makes sense to path integral by time-sliced approximation.

Now, for the proof of Lemma A, we content ourselves with only confirming applicability of the Chernoff's theorem on $\mathbf{X} = L^2(\mathbf{R}^d)$ with $L = H^{(1)} - m$, and (3.6), i.e.

$$(3.11) \quad (F(t)g)(x) := \int_{\mathbf{R}^d} (e^{-t[\sqrt{-\Delta+m^2}-m]})(x-y) e^{iA(\frac{x+y}{2})(y-x)-V(\frac{x+y}{2})t} g(y) dy,$$

where we are writing the integral kernel $k_0(t, x - y)$ of the semigroup $e^{-t[\sqrt{-\Delta+m^2}-m]}$ as $(e^{-t[\sqrt{-\Delta+m^2}-m]})(x - y)$.

Indeed, we can show that $\frac{I-F(t)}{t} \rightarrow H^{(1)}$ in strong resolvent sense as $t \downarrow 0$, which yields Lemma A, namely, that LHS of (3.10) converges to $e^{-t[H^{(1)}-m]}g$ as $n \rightarrow \infty$. \square

Proof of convergence of RHS of (3.10). We are going to show

$$\begin{aligned} \text{RHS of (3.10)} &= \int_{D_x} e^{-S_n(X)} g(X(t)) d\lambda_x(X) \\ &= \int_{D_x} e^{-i \sum_{j=1}^n A\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \cdot (X(t_j)-X(t_{j-1})) - \sum_{j=1}^n V\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \frac{t}{n}} \\ &\quad \times g(X(t)) d\lambda_x(X) \\ &\rightarrow \int_{D_x} e^{-S(X)} g(X(t)) d\lambda_x(X), \quad \text{as } n \rightarrow \infty. \end{aligned}$$

In fact, in equation (3.8), we can use *Itô's formula* [IkW-81,89] for the j -th summand of the first term on the right to rewrite it as a sum of three integrals on the t -interval $t_{j-1} \leq s < t_j$:

$$\begin{aligned} &A\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \cdot (X(t_j) - X(t_{j-1})) \\ &= \int_{t_{j-1}}^{t_j+} \int_{|y|>0} \left[A\left(\frac{X(s-)+X(t_{j-1})+yI_{|y|\geq 1}(y)}{2}\right) \cdot (X(s-) - X(t_{j-1}) + yI_{|y|\geq 1}(y)) \right. \\ &\quad \left. - A\left(\frac{X(s-)+X(t_{j-1})}{2}\right) \cdot (X(s-) - X(t_{j-1})) \right] N_X(dsdy) \\ &\quad + \int_{t_{j-1}}^{t_j+} \int_{|y|>0} \left[A\left(\frac{X(s-)+X(t_{j-1})+yI_{|y|<1}(y)}{2}\right) \cdot (X(s-) - X(t_{j-1}) + yI_{|y|<1}(y)) \right. \\ &\quad \left. - A\left(\frac{X(s-)+X(t_{j-1})}{2}\right) \cdot (X(s-) - X(t_{j-1})) \right] \tilde{N}(dsdy) \\ &\quad + \int_{t_{j-1}}^{t_j} \int_{|y|>0} \left[A\left(\frac{X(s)+X(t_{j-1})+yI_{|y|<1}(y)}{2}\right) \cdot (X(s) - X(t_{j-1}) + yI_{|y|<1}(y)) \right. \\ &\quad \left. - A\left(\frac{X(s)+X(t_{j-1})}{2}\right) \cdot (X(s) - X(t_{j-1})) \right. \\ &\quad \left. - I_{|y|<1}(y) \left(\left(\frac{1}{2}(y \cdot \nabla) A \right) \left(\frac{X(s)+X(t_{j-1})}{2} \right) \cdot (X(s) - X(t_{j-1})) + y \cdot A\left(\frac{X(s)+X(t_{j-1})}{2}\right) \right) \right] ds n(dy) \end{aligned}$$

It follows that

$$\begin{aligned} S_n(X) &= i \sum_{j=1}^n A\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \cdot (X(t_j) - X(t_{j-1})) + \sum_{j=1}^n V\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \frac{t}{n} \\ &= \sum_{j=1}^n \left[i \int_{t_{j-1}}^{t_j+} \int_{|y|>0} \cdots N_X(dsdy) + i \int_{t_{j-1}}^{t_j+} \int_{|y|>0} \cdots \tilde{N}(dsdy) \right. \\ &\quad \left. + i \int_{t_{j-1}}^{t_j} \int_{|y|>0} \cdots ds n(dy) + V\left(\frac{X(t_{j-1})+X(t_j)}{2}\right) \frac{t}{n} \right], \end{aligned}$$

which, as $n \rightarrow \infty$, converges to

$$\begin{aligned} & i \left[\int_0^{t+} \int_{|y| \geq 1} A(X(s-) + \frac{y}{2}) \cdot y N_X(ds dy) + \int_0^{t+} \int_{0 < |y| < 1} A(X(s-) + \frac{y}{2}) \cdot y \tilde{N}_X(ds dy) \right. \\ & \quad \left. + \int_0^t ds \text{ p.v.} \int_{0 < |y| < 1} A(X(s) + \frac{y}{2}) \cdot y n(dy) \right] + \int_0^t V(X(s)) ds \\ & \equiv S^{(1)}(t, X), \end{aligned}$$

whence

$$\text{RHS of (3.10)} = \int_{D_x} e^{-S_n(X)} g(X(t)) d\lambda_x(X) \rightarrow \int_{D_x} e^{-S^{(1)}(t, X)} g(X(t)) d\lambda_x(X).$$

□

§ 3.2. The case for the Weyl pseudo-differential operator modified by Iftimie–Măntoiu–Purice $H^{(2)} := H_A^{(2)} + V$

First note that we can rewrite $H_A^{(2)}$, in (2.2), similarly for $H_A^{(1)}$, as integral operator

$$\begin{aligned} (3.12) \quad ([H_A^{(2)} - m]f)(x) &= - \int_{|y| > 0} [e^{-iy \cdot \int_0^1 A(x+\theta y) d\theta} f(x+y) - f(x) \\ & \quad - I_{\{|y| < 1\}} y \cdot (\nabla - iA(x)) f(x)] n(dy) \\ &= - \lim_{r \downarrow 0} \int_{|y| \geq r} [e^{-iy \cdot \int_0^1 A(x+\theta y) d\theta} f(x+y) - f(x)] n(dy) \\ &= - \text{p.v.} \int_{|y| > 0} [e^{-iy \cdot \int_0^1 A(x+\theta y) d\theta} f(x+y) - f(x)] n(dy). \end{aligned}$$

Theorem 3.2. [IfMP-07, 08, 10]

$$\begin{aligned} (3.13) \quad (e^{-t[H^{(2)} - m]}g)(x) &= \int_{D_x([0, \infty) \rightarrow \mathbf{R}^d)} e^{-S^{(2)}(t, X)} g(X(t)) d\lambda_x(X), \\ S^{(2)}(t, X) &= i \int_0^{t+} \int_{|y| \geq 1} \left(\int_0^1 A(X(s-) + \theta y) \cdot y d\theta \right) N_X(ds dy) \\ & \quad + i \int_0^{t+} \int_{0 < |y| < 1} \left(\int_0^1 A(X(s-) + \theta y) \cdot y d\theta \right) \tilde{N}_X(ds dy) \\ & \quad + i \int_0^t ds \text{ p.v.} \int_{0 < |y| < 1} \left(\int_0^1 A(X(s) + \theta y) \cdot y d\theta \right) n(dy) \\ & \quad + \int_0^t V(X(s)) ds. \end{aligned}$$

The proof of Theorem 3.2 is the same as that of Theorem 3.1. We have only to replace $A(X(s-) + \frac{y}{2}) \cdot y$ by $\int_0^1 A(X(s-) + \theta y) \cdot y d\theta$ and consider

$$(3.14) \quad (F(t)g)(y) := \int_{\mathbf{R}^d} (e^{-t[\sqrt{-\Delta+m^2}-m]})(x-y) e^{[-i(y-x) \int_0^1 A((1-\theta)y+\theta x)d\theta - V(y)t]} g(y) dy,$$

for which note the second expression of the definition (2.2) of $H_A^{(2)}$. Etc.

§ 3.3. The case for $H^{(3)} := H_A^{(3)} + V$

The kinetic part $H_A^{(3)}$ is defined by operator-theoretical square root of the Schrödinger operator $S := 2H_A^{NR} + m^2$, $H_A^{NR} := \frac{1}{2}(-i\nabla - A(x))^2$. We can say all information of $H_A^{(3)}$ is contained in $S := 2H_A^{NR} + m^2$ or the *nonrelativistic magnetic Schrödinger operator* H_A^{NR} . So the problem is how to extract the information from it. For instance, the corresponding semigroup $e^{-t(H_A^{(3)}-m)}$ is completely determined by H_A^{NR} through theory of fractional powers [Y, Chap.IX, 11, pp.259–261] as

$$e^{-t[H_A^{(3)}-m]}g = \begin{cases} e^{mt} \int_0^\infty f_t(\lambda) e^{-\lambda[2H_A^{NR}+m^2]} g d\lambda, & t > 0, \\ 0, & t = 0 \end{cases}$$

$$f_t(\lambda) = \begin{cases} (2\pi i)^{-1} \int_{\sigma-i\infty}^{\sigma+i\infty} e^{z\lambda-tz^{1/2}} dz, & \lambda \geq 0, \\ 0, & \lambda < 0 \quad (\sigma > 0). \end{cases}$$

Here $e^{-\lambda[2H_A^{NR}+m^2]}$ is represented by the Feynman–Kac–Itô formula, but we don't do it.

Instead, we note there is probabilistic counterpart of the above procedure of going from Wiener process (\equiv nonrelativistic Schrödinger) to Lévy process (\equiv (square root) relativistic Schrödinger). It is *subordination* (by Bochner).

In this context, the problem of path integral for $e^{-t[H^{(3)}-m]}g$ was studied first by DeAngelis, Serva and Rinaldi [AnSe-90], [AnRSe-91], then by [N-96, 97, 00] with use of *subordination* of Brownian motion, and recently more extensively by Hiroshima–Ichinose–Lőrinczi [HILo-12, 13] (cf. [LoHB-11]) not only for magnetic relativistic Schrödinger operator but also for *Bernstein functions* of magnetic nonrelativistic Schrödinger operator even with spin.

Now, what is *subordination*?

Start with the 1-dimensional *standard* Brownian motion $B^1(t) \in C_0([0, \infty) \rightarrow \mathbf{R})$ with $B^1(0) = 0$ and μ_0 the Wiener measure on $C_0([0, \infty) \rightarrow \mathbf{R})$ such that $e^{-t\frac{1}{2}\xi^2} = \int_{C_0([0, \infty) \rightarrow \mathbf{R})} e^{iB^1(t)\xi} d\mu_0(B^1)$, then put

$$(3.15) \quad T(t) := \inf\{s > 0; B^1(s) + ms = t\}, \quad t \geq 0.$$

Then $T(t)$ becomes a monotone, non-decreasing function on $[0, \infty)$ with $T(0) = 0$, belonging to $D_0([0, \infty) \rightarrow \mathbf{R})$, so that it is a 1-dimensional Lévy process. This $T(t)$ is what is called *subordinator* ([Sa-99, Chap.6, p.197], cf. [Sa-90]; [Ap-09, 1.3.2, p.52]), which gives *time change*. Let ν_0 be the probability measure of the associated process on space $D_0([0, \infty) \rightarrow \mathbf{R})$.

Lemma B. (e.g. [Ap-09, p.54, Example 1.3.21, p.54, and Exercise 2.1.10, p.96; cf. Theorem 2.2.9, p.95])

$$(3.16) \quad e^{-t[\sqrt{2\sigma+m^2}-m]} = \int_{D_0([0, \infty) \rightarrow \mathbf{R})} e^{-T(t)\sigma} d\nu_0(T), \quad \sigma \geq 0$$

We are in a position to give a path integral representation for $e^{-t[H^{(3)}-m]}g$.

Theorem 3.3. ([AnSe-90], [AnRSe-91], [N-96, 97, 00]; [HILo-12]).

$$(3.17) \quad (e^{-t[H^{(3)}-m]}g)(x) = \int \int_{\substack{C_x([0, \infty) \rightarrow \mathbf{R}^d) \\ \times D_0([0, \infty) \rightarrow \mathbf{R})}} e^{-S^{(3)}(t, B, T)} g(B(T(t))) d\mu_x(B) d\nu_0(T),$$

$$S^{(3)}(t, B, T) = i \int_0^{T(t)} A(B(s)) dB(s) + \frac{i}{2} \int_0^{T(t)} \operatorname{div} A(B(s)) ds$$

$$+ \int_0^t V(B(T(s))) ds,$$

$$\equiv i \int_0^{T(t)} A(B(s)) \circ dB(s) + \int_0^t V(B(T(s))) ds$$

Here $C_x([0, \infty) \rightarrow \mathbf{R}^d)$ is the set of continuous paths (Brownian motions) $B : [0, \infty) \rightarrow \mathbf{R}^d$ with $B(0) = x$, and μ_x is the Wiener measure on $C_x([0, \infty) \rightarrow \mathbf{R}^d)$:

$$\exp \left[-t \frac{\xi^2}{2} \right] = \int_{C_x([0, \infty) \rightarrow \mathbf{R}^d)} e^{i(B(t)-x) \cdot \xi} d\mu_x(B) \quad (m > 0)$$

Before going to proof of Theorem 3.3, recall the Feynman–Kac–Itô formula [e.g. S-05] for the magnetic nonrelativistic Schrödinger operator $H^{NR} := H_A^{NR} + V := \frac{1}{2}(-i\nabla - A(x))^2 + V(x)$:

$$(3.18) \quad (e^{-tH^{NR}}g)(x)$$

$$= \int_{C_x([0, \infty) \rightarrow \mathbf{R}^d)} e^{-[i \int_0^t A(B(s)) dB(s) + \frac{i}{2} \int_0^t \operatorname{div} A(B(s)) ds + \int_0^t V(B(s)) ds]} g(B(t)) d\mu_x(B)$$

$$\equiv \int_{C_x([0, \infty) \rightarrow \mathbf{R}^d)} e^{-[i \int_0^t A(B(s)) \circ dB(s) + \int_0^t V(B(s)) ds]} g(B(t)) d\mu_x(B) \quad (\text{Stratonovich})$$

Proof of Theorem 3.3 (Sketch). We use Lemma B, the spectral theorem for selfadjoint operator and Feynman–Kac–Itô formula above. Note that $H_A^{(3)} = \sqrt{2H_A^{NR} + m^2}$. $\langle \cdot, \cdot \rangle$

stands the inner product of Hilbert space $L^2(\mathbf{R}^2)$. By spectral theorem for the selfadjoint operator H_A^{NR} (magnetic nonrelativistic Schrödinger operator with $V = 0$), we have $H_A^{NR} = \int_{\text{Spec}(H_A^{NR})} \sigma dE(\sigma)$. Then for $f, g \in L^2(\mathbf{R}^d)$

$$\langle f, e^{-t[H_A^{(3)} - m]} g \rangle = \int_{\text{Spec}(H_A^{NR})} e^{-t[\sqrt{2\sigma + m^2} - m]} \langle f, dE(\sigma) g \rangle$$

By Lemma B and again by spectral theorem,

$$\begin{aligned} \langle f, e^{-t[H_A^{(3)} - m]} g \rangle &= \int_{\text{Spec}(H_A^{NR})} \int_{D_0([0, \infty) \rightarrow \mathbf{R})} e^{-T(t)\sigma} d\nu_0(T) \langle f, dE(\sigma) g \rangle \\ &= \int_{D_0([0, \infty) \rightarrow \mathbf{R})} \langle f, e^{-T(t)H_A^{NR}} g \rangle d\nu_0(T). \end{aligned}$$

Applying Feynman–Kac–Itô (with $V = 0$) to $e^{-T(t)H_A^{NR}} g$ on the right-hand side,

$$\begin{aligned} &\langle f, e^{-t[H_A^{(3)} - m]} g \rangle \\ &= \int_{D_0([0, \infty) \rightarrow \mathbf{R})} d\nu_0(T) \int_{\mathbf{R}^d} dx \overline{f(B(0))} \int_{C_x([0, \infty) \rightarrow \mathbf{R}^d)} e^{-i \int_0^{T(t)} A(B(s)) \odot dB(s)} g(B(T(t))) d\mu_x(B) \\ &= \int_{\mathbf{R}^d} dx \overline{f(x)} \int_{D_0([0, \infty) \rightarrow \mathbf{R})} \int_{C_x([0, \infty) \rightarrow \mathbf{R}^d)} e^{-i \int_0^{T(t)} A(B(s)) \odot dB(s)} g(B(T(t))) d\nu_0(T) d\mu_x(B) \end{aligned}$$

Here note $B(0) = x$. This proves the assertion when $V = 0$.

When $V \neq 0$, with partition of $[0, t]$: $0 = t_0 < t_1 < \dots < t_n = t$, $t_j - t_{j-1} = t/n$, we can express $e^{-t[H_A^{(3)} - m]} g = e^{-t[(H_A^{(3)} - m) + V]}$ by Trotter–Kato formula or by Chernoff’s theorem with $F(t) := e^{-t[H_A^{(3)} - m]} e^{-tV}$,

$$e^{-t[H_A^{(3)} - m]} g = \lim_{n \rightarrow \infty} (e^{-(t/n)[H_A^{(3)} - m]} e^{-(t/n)V})^n g,$$

where convergence on the right-hand side is in strong sense. Rewrite these n operators product by path integral on probability product measure $\nu_0(T) \cdot \mu_x(B)$, then we have (recall $T(0) = T(t_0) = 0$, $B(0) = B(T(t_0)) = x$),

$$\begin{aligned} &\langle f, (e^{-(t/n)[H_A^{(3)} - m]} e^{-(t/n)V})^n g \rangle \\ &= \int_{\mathbf{R}^d} dx \int_{D_0([0, \infty) \rightarrow \mathbf{R})} d\nu_0(T) \int_{C_x([0, \infty) \rightarrow \mathbf{R}^d)} \overline{f(B(0))} \\ &\quad \times e^{-i \sum_{j=1}^n \int_{T(t_{j-1})}^{T(t_j)} A(B(s)) \odot dB(s)} e^{-\sum_{j=1}^n V(B(T(t_j))) \frac{t}{n}} g(B(t_n)) d\mu_x(B) \end{aligned}$$

We see, as $n \rightarrow \infty$, that LHS converges to $\langle f, e^{-t[H_A^{(3)} - m]} g \rangle$, and the right-hand side also converges to the goal formula as integral by the product measure $dx \cdot \nu_0(T) \cdot \mu_x(B)$,

through Lebesgue theorem. This shows the weak convergence. The strong convergence will also be shown. \square

§ 3.4. Summary of three path integral formulas

Finally, as summary, we will collect the three path integral representation formulas in Theorems 3.1, 3.2, 3.3, below, so as to be able to easily see x -dependence. To do so, make change of space, probability measure and paths by translation:

$D_x \rightarrow D_0$, $\lambda_x \rightarrow \lambda_0$, $X(s) \rightarrow X(s) + x$, $B(s) \rightarrow B(s) + x$, $B(T(s)) \rightarrow B(T(s)) + x$, then

$$\begin{aligned}
 (3.5) : (e^{-t[H^{(1)}-m]}g)(x) &= \int_{D_0([0,\infty) \rightarrow \mathbf{R}^d)} e^{-S^{(1)}(t,X)} g(X(t) + x) d\lambda_0(X), \\
 S^{(1)}(t, X) &= i \int_0^{t+} \int_{|y| \geq 1} A(X(s-) + x + \frac{y}{2}) \cdot y N_X(dsdy) \\
 &\quad + i \int_0^{t+} \int_{0 < |y| < 1} A(X(s-) + x + \frac{y}{2}) \cdot y \tilde{N}_X(dsdy) \\
 &\quad + i \int_0^t ds \text{ p.v.} \int_{0 < |y| < 1} A(X(s) + x + \frac{y}{2}) \cdot y n(dy) + \int_0^t V(X(s) + x) ds; \\
 (3.12) : (e^{-t[H^{(2)}-m]}g)(x) &= \int_{D_0([0,\infty) \rightarrow \mathbf{R}^d)} e^{-S^{(2)}(t,X)} g(X(t) + x) d\lambda_0(X), \\
 S^{(2)}(t, X) &= i \int_0^{t+} \int_{|y| \geq 1} \left(\int_0^1 A(X(s-) + x + \theta y) \cdot y d\theta \right) N_X(dsdy) \\
 &\quad + i \int_0^{t+} \int_{0 < |y| < 1} \left(\int_0^1 A(X(s-) + x + \theta y) \cdot y d\theta \right) \tilde{N}_X(dsdy) \\
 &\quad + i \int_0^t ds \text{ p.v.} \int_{0 < |y| < 1} \left(\int_0^1 A(X(s) + x + \theta y) \cdot y d\theta \right) n(dy) + \int_0^t V(X(s) + x) ds; \\
 (3.17) : (e^{-t[H^{(3)}-m]}g)(x) &= \int_{\substack{C_0([0,\infty) \rightarrow \mathbf{R}^d) \\ \times D_0([0,\infty) \rightarrow \mathbf{R})}} e^{-S^{(3)}(t,B,T)} g(B(T(t)) + x) d\mu_0(B) d\nu_0(T), \\
 S^{(3)}(t, B, T) &= i \int_0^{T(t)} A(B(s) + x) \cdot dB(s) + \frac{i}{2} \int_0^{T(t)} \text{div} A(B(s) + x) ds + \int_0^t V(B(T(s)) + x) ds, \\
 &\equiv i \int_0^{T(t)} A(B(s) + x) \circ dB(s) + \int_0^t V(B(T(s)) + x) ds
 \end{aligned}$$

§ 3.5. Path integral formulas (3.5), (3.12) and (3.15) as time-sliced approximation

In the proof of path integral formula (3.5) in Theorem 3.1, we have used Chernoff's theorem to show Lemma A, i.e. that $F(t/n)^n g$, the left-hand side of equality (3.10) converges to $e^{-tH^{(1)}} g$, the left-hand side of (3.5). We are now going to see how $F(t)$ in (3.6)/(3.11) comes out heuristically for L being the relativistic Schrödinger operators $H^{(1)} = H_A^{(1)} + V$, $H^{(1)} = H_A^{(1)} + V$, but there is a different situation for $H^{(3)} = H_A^{(3)} + V$. For the details, we refer to [I-13, §4.2].

We use in what follows the time-sliced approximation, with partition of the interval $[0, t]$ into n small subintervals: $0 = t_0 < t_1 < \cdots < t_n = t$, only with *equal width* t/n , $t_j - t_{j-1} = t/n$, $1 \leq j \leq n$.

(1) For $L = H^{(1)} = H_A^{(1)} + V$. The second member of (3.10) can be heuristically rewritten by the *imaginary-time phase space path integral* ([G-66], [M-78]) through time-sliced approximation, i.e. as the $n \rightarrow \infty$ limit of the integral

$$\begin{aligned}
& \overbrace{\int_{\mathbf{R}^{2d}} \cdots \int_{\mathbf{R}^{2d}}}^{n \text{ times}} e^{i \sum_{l=1}^n (X(t_l) - X(t_{l-1})) \cdot \Xi(X(t_{l-1}))} \\
& \quad \times e^{-\frac{t}{n} \sum_{l=1}^n \left[\sqrt{\left(\Xi(t_{l-1}) - A\left(\frac{X(t_{l-1}) + X(t_l)}{2}\right) \right)^2 + m^2} - m + V(X(t_{l-1})) \right]} \\
& \quad \times g(X(0)) \prod_{j=1}^n \frac{d\Xi(t_{j-1}) dX(t_{j-1})}{(2\pi)^d} \\
& = \overbrace{\int_{\mathbf{R}^{2d}} \cdots \int_{\mathbf{R}^{2d}}}^{n \text{ times}} e^{i \sum_{l=1}^n (X(t_l) - X(t_{l-1})) \cdot \left(\Xi(t_{l-1}) + A\left(\frac{X(t_{l-1}) + X(t_l)}{2}\right) \right)} \\
& \quad \times e^{-\frac{t}{n} \sum_{l=1}^n \left[\sqrt{\Xi(t_{l-1})^2 + m^2} - m + V(X(t_{l-1})) \right]} g(X(0)) \prod_{j=1}^n \frac{d\Xi(t_{j-1}) dX(t_{j-1})}{(2\pi)^d} \\
& = \overbrace{\int_{\mathbf{R}^{2d}} \cdots \int_{\mathbf{R}^{2d}}}^{n \text{ times}} e^{\sum_{l=1}^n \left\{ i(x_l - x_{l-1}) \cdot \left(\xi_{l-1} + A\left(\frac{X(t_{l-1}) + X(t_l)}{2}\right) \right) - \frac{t}{n} \left[\sqrt{\xi_{l-1}^2 + m^2} - m + V(x_{l-1}) \right] \right\}} \\
& \quad \times g(x_0) \prod_{j=1}^n \frac{d\xi_{j-1} dx_{j-1}}{(2\pi)^d}, \tag{3.19}
\end{aligned}$$

where, in the first equality, we made *change of variables*: $\Xi'(\cdot) := \Xi(\cdot) + A(X(\cdot))$, $X'(\cdot) := X(\cdot)$ on the space of phase space paths, and then written $\Xi(\cdot)$, $X(\cdot)$ again for $\Xi'(\cdot)$, $X'(\cdot)$. In the second equality, we put $\xi_j = \Xi(t_j)$, $x_j = X(t_j)$, $j = 0, 1, \dots, n-1$, and $x = x_n = X(t_n) = X(t)$. Notice that here the assignment $t_j \mapsto (\Xi(t_j), X(t_j))$ differs from the one used for (3.8). This is chronological, while that was anti-chronological. Equation (3.19) is suggesting us how that functional of the path $X(\cdot)$, which is to be created as $e^{-S^{(1)}(t,x)}$ in (3.5) by the approximation $F(t/n)^n$, does look.

Then the last member of (3.19) can be rewritten as

$$\begin{aligned}
& \overbrace{\int_{\mathbf{R}^{2d}} \cdots \int_{\mathbf{R}^{2d}}}^{n \text{ times}} \prod_{l=1}^n \left\{ \left[e^{i(x_l - x_{l-1}) \cdot \xi_{l-1}} e^{-\frac{t}{n} [\sqrt{\xi_{l-1}^2 + m^2} - m]} \right] \right. \\
& \quad \left. \times e \left[iA \left(\frac{x_{l-1} + x_l}{2} \right) \cdot (x_l - x_{l-1}) - V \left(\frac{x_{l-1} + x_l}{2} \right) \frac{t}{n} \right] \right\} g(x_0) \prod_{j=1}^n \frac{d\xi_{j-1} dx_{j-1}}{(2\pi)^d} \\
& = \overbrace{\int_{\mathbf{R}^d} \cdots \int_{\mathbf{R}^d}}^{n \text{ times}} \prod_{l=1}^n \left\{ \left[e^{-\frac{t}{n} [\sqrt{-\Delta + m^2} - m]} \right] (x_l - x_{l-1}) \right. \\
& \quad \left. \times e \left[iA \left(\frac{x_{l-1} + x_l}{2} \right) \cdot (x_l - x_{l-1}) - V \left(\frac{x_{l-1} + x_l}{2} \right) \frac{t}{n} \right] \right\} g(x_0) dx_0 dx_1 \cdots dx_{n-1},
\end{aligned} \tag{3.20}$$

with $x = x_n$, where we have performed all the $d\xi_j$ integrations. The result is nothing but $F(t/n)^n g$ in (3.10) with $F(t)$ in (3.7).

(2) For $L = H^{(2)} = H_A^{(2)} + V$. Similar treatment is valid for $L = H^{(2)} = H_A^{(2)} + V$, where we may consider for $H^{(2)}$ with

$$\int_0^1 A((1-\theta)X(t_{l-1}) + \theta X(t_l)) d\theta$$

in place of

$$A\left(\frac{X(t_{l-1}) + X(t_l)}{2}\right)$$

for $H^{(1)}$ on each subinterval $[t_{j-1}, t_j]$. The same arguments as for $L = H^{(1)}$ above will show the expression (3.12) is also obtained heuristically through time-sliced approximation with $F(t)$ in (3.14).

(3) For $H^{(3)} = H_A^{(3)} + V$. In this case, formula (3.17) does not seem to be one which can be heuristically obtained, probably because $H_A^{(3)}$ cannot be so explicitly well expressed by a pseudo-differential operator defined through a certain *tractable symbol* as $H_A^{(1)}$ and $H_A^{(2)}$.

Indeed, for the semigroups $e^{-t[H_A^{(1)} + V]}$ and $e^{-t[H_A^{(2)} + V]}$, take (3.7)/(3.11) as $F(t)$, we could show that $F(t/n)^n \rightarrow e^{-t[H_A^{(j)} + V]}$ strongly for $j = 1, 2$. But for the semigroup $e^{-t[H_A^{(3)} + V]}$, such an interpretation does not seem possible.

§ 4. Some observation on Chernoff's theorem and path integral by time-sliced approximation

It is well-known that, for the solution of Schrödinger equation, the Trotter–Kato product formula can simply and plainly give a, though naive, meaning to its path

integral representation by *time-sliced approximation*, if the Schrödinger operator has no *magnetic vector potential* but only electric scalar potential $V(x)$. However, if it has also *magnetic vector potential* $A(x)$, it does not seem to go well, and then we need Chernoff's theorem. Our aim is to observe how useful and effective a tool Chernoff's theorem is to give a meaning to path integral formulas by *time-sliced approximation*, guaranteeing its convergence. For this aspect, we also refer to [BoBuScSm-11].

For our convenience, we begin this section with restating the Chernoff's theorem, though already done in §3.1. Notice that Trotter–Kato product formula follows from Chernoff's theorem, but the converse is not valid.

Chernoff's Theorem. [Ch-74] *Let F be a strongly continuous function on $[0, \infty)$ with values in the Banach space $\mathcal{L}(\mathbf{X})$ of bounded linear operators on a Banach space \mathbf{X} . Assume that F further satisfies the following conditions: (i) $F(0) = I$ (I : identity operator on \mathbf{X}), and there exists a real a such that $\|F(t)\| \leq e^{at}$ for all $t \geq 0$; (ii) The linear operator $F'(0) \upharpoonright_{D[F'(0)]}$ is closable, and the closure $\overline{F'(0)} := L$ generates a strongly continuous semigroup e^{-tL} .*

Then $F(t/n)^n$ converges to e^{-tL} strongly, as $n \rightarrow \infty$, uniformly on each finite interval in $t \geq 0$.

The content of this section is almost independent of the three relativistic Schrödinger operators $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$ and their path integral representation formulas, about which we have already discussed enough up to the previous section §3. In this section, we will study further this wisdom with several other evolution equations in quantum mechanics to watch their corresponding path integral representation formulas. We first treat the case of strong convergence and next the case of convergence in norm and/or pointwise for the integral kernels.

Throughout this section again, the time-sliced approximation, with partition of the interval $[0, t]$ into n small subintervals: $0 = t_0 < t_1 < \cdots < t_n = t$, is used only with equal width t/n , $t_j - t_{j-1} = t/n$, $1 \leq j \leq n$.

§ 4.1. Time-sliced approximation in strong topology

We consider, first, the time-sliced approximation for the solution of Schrödinger equation in real and/or imaginary time, only with scalar potential, that is, *without magnetic vector potential*, and see it strongly converge by Trotter–Kato product formula as well as Chernoff's theorem. Next, we come to consider the Schrödinger equation and Dirac equation *in presence of magnetic vector potential* and realize in turn to need to use Chernoff's theorem.

4.1.1. Schrödinger operator with scalar potential $V(x)$

The operator concerned is $H_V := -\frac{1}{2}\Delta + V$ in $L^2(\mathbf{R}^3)$. Put

$$(4.1) \quad (F(t)g)(x) := (e^{-it(-\frac{1}{2}\Delta)}e^{-itV})(x) = \int [e^{-it(-\frac{1}{2}\Delta)}](x-y)e^{-itV(y)}g(y)dy,$$

$$(4.2) \quad (G(t)g)(x) := (e^{-t(-\frac{1}{2}\Delta)}e^{-tV}g)(x) = \int [e^{-t(-\frac{1}{2}\Delta)}](x-y)e^{-tV(y)}g(y)dy,$$

where $[e^{-it(-\frac{1}{2}\Delta)}](x-y)$ and $[e^{-t(-\frac{1}{2}\Delta)}](x-y)$ stand for the integral kernels of the Schrödinger unitary group $e^{-it(-\frac{1}{2}\Delta)}$ and Schrödinger semigroup $e^{-t(-\frac{1}{2}\Delta)}$, respectively.

Under certain reasonable conditions on $V(x)$, it holds in strong resolvent sense in $L^2(\mathbf{R}^3)$ as $t \downarrow 0$ that $\frac{I-F(t)}{t}$ converges to iH_V , while $\frac{I-G(t)}{t}$ converges to H_V . Then by Chernoff's theorem or in this case by Trotter–Kato product formula, we have, for $g \in L^2(\mathbf{R}^3)$,

$$(4.3) \quad F(t/n)^n g \rightarrow e^{-it[-\frac{1}{2}\Delta+V]}g, \quad \text{strongly},$$

$$(4.4) \quad G(t/n)^n g \rightarrow e^{-t[-\frac{1}{2}\Delta+V]}g, \quad \text{strongly},$$

as $n \rightarrow \infty$. On the other hand, $e^{-it[-\frac{1}{2}\Delta+V]}g$ should be given by the *configuration space path integral* through time-sliced approximation as the $n \rightarrow \infty$ limit of the integral

$$(4.5) \quad \begin{aligned} & C_n \overbrace{\int_{\mathbf{R}^d} \cdots \int_{\mathbf{R}^d}}^{n \text{ times}} e^{i \sum_{l=1}^n \left[\frac{1}{2} \left(\frac{X(t_l) - X(t_{l-1})}{t/n} \right)^2 - V(X(t_{l-1})) \right] \frac{t}{n}} g(X(0)) \prod_{j=1}^n d(X(t_{j-1})) \\ &= C_n \overbrace{\int_{\mathbf{R}^d} \cdots \int_{\mathbf{R}^d}}^{n \text{ times}} \prod_{j=1}^n \left[e^{i \frac{t}{n} \frac{1}{2} \left(\frac{x_j - x_{j-1}}{t/n} \right)^2} e^{-i \frac{t}{n} V(x_{j-1})} \right] g(x_0) dx_0 dx_1 \cdots dx_{n-1}, \end{aligned}$$

with some renormalization constant C_n depending on t , where we put $x_j = X(t_j)$, $j = 0, 1, \dots, n-1$, and $x = x_n = X(t_n) = X(t)$. Taking $C_n = \left(\frac{i}{2\pi t/n}\right)^{3n/2}$, this is what is meant by $F(t/n)^n g$.

Similarly, $e^{-t[-\frac{1}{2}\Delta+V]}g$ should be given by the *configuration space imaginary-time path integral* through time-sliced approximation as the $n \rightarrow \infty$ limit of the integral

$$(4.6) \quad \begin{aligned} & C'_n \overbrace{\int_{\mathbf{R}^d} \cdots \int_{\mathbf{R}^d}}^{n \text{ times}} e^{-\sum_{l=1}^n \left[\frac{1}{2} \left(\frac{X(t_l) - X(t_{l-1})}{t/n} \right)^2 + V(X(t_{l-1})) \right] \frac{t}{n}} g(X(0)) \prod_{j=1}^n d(X(t_{j-1})) \\ &= C'_n \overbrace{\int_{\mathbf{R}^d} \cdots \int_{\mathbf{R}^d}}^{n \text{ times}} \prod_{j=1}^n \left[e^{-\frac{t}{n} \frac{1}{2} \left(\frac{x_j - x_{j-1}}{t/n} \right)^2} e^{-\frac{t}{n} V(x_{j-1})} \right] g(x_0) dx_0 dx_1 \cdots dx_{n-1}, \end{aligned}$$

with some renormalization constant C'_n depending on t , where put $x_j = X(t_j)$, $j = 0, 1, \dots, n-1$, and $x = x_n = X(t_n) = X(t)$. Taking $C'_n = (\frac{1}{2\pi t/n})^{3n/2}$, this is what is meant by $G(t/n)^n g$.

4.1.2. Schrödinger operator with vector and scalar potentials $A(x)$ and $V(x)$

The operator concerned is $H_{A,V} := \frac{1}{2}(-i\nabla - A(x))^2 + V$ in $L^2(\mathbf{R}^3)$. Put

$$(4.7) \quad (F(t)g)(x) := \int [e^{-it\frac{1}{2}(-\Delta)}](x-y)e^{i[A(\frac{x+y}{2})(x-y)-V(\frac{x+y}{2})t]}g(y)dy;$$

$$(4.8) \quad (G(t)g)(x) := \int [e^{-t\frac{1}{2}(-\Delta)}](x-y)e^{iA(\frac{x+y}{2})(x-y)-V(\frac{x+y}{2})t}g(y)dy.$$

Then, under certain reasonable conditions on $A(x)$ and $V(x)$, though one cannot use Trotter–Kato product formula because of presence of the vector potential $A(x)$, we have by Chernoff's theorem instead that as $n \rightarrow \infty$,

$$(4.9) \quad F(t/n)^n g \rightarrow e^{-it[\frac{1}{2}(-i\nabla - A(x))^2 + V]}g, \quad \text{strongly,}$$

$$(4.10) \quad G(t/n)^n g \rightarrow e^{-t[\frac{1}{2}(-i\nabla - A(x))^2 + V]}g, \quad \text{strongly.}$$

On the other hand, $e^{-it[\frac{1}{2}(-i\nabla - A(x))^2 + V]}g$ should be given by the *phase space path integral* ([G-66], [M-78]) through time-sliced approximation. We make the same argument for $H_{A,V}$ as used in (3.19) through (3.20) for the relativistic Schrödinger operator $H^{(1)} = H_A^{(1)} + V$, but here (and also below in §4.2.3), for simplicity, by skipping the step of performing the change of variables (on the space of phase space paths) inside (3.19). Then $e^{-it[\frac{1}{2}(-i\nabla - A(x))^2 + V]}g$ should be reached as the $n \rightarrow \infty$ limit of the integral

$$\begin{aligned} (4.11) \quad & \overbrace{\int_{\mathbf{R}^{2d}} \cdots \int_{\mathbf{R}^{2d}}}^{n \text{ times}} e^{i \sum_{l=1}^n [(X(t_l) - X(t_{l-1})) \cdot \Xi(t_{l-1}) - \frac{t}{n} \frac{\Xi(t_{l-1})^2}{2}]} \\ & \times e^{i \sum_{l=1}^n [A(\frac{X(t_l) + X(t_{l-1})}{2}) \cdot (X(t_l) - X(t_{l-1})) - \frac{t}{n} V(X(t_{l-1}))]} g(X(0)) \prod_{j=1}^n \frac{d\Xi(t_{j-1}) dX(t_{j-1})}{(2\pi)^3} \\ & = \overbrace{\int_{\mathbf{R}^{2d}} \cdots \int_{\mathbf{R}^{2d}}}^{n \text{ times}} \prod_{j=1}^n \left\{ e^{[i(x_j - x_{j-1}) \cdot \xi_{j-1} - i \frac{t}{n} \frac{\xi_{j-1}^2}{2}]} e^{[A(\frac{x_j + x_{j-1}}{2}) \cdot (x_j - x_{j-1}) - \frac{t}{n} V(x_{j-1})]} \right\} g(x_0) \\ & \quad \times \frac{d\xi_0 dx_0}{(2\pi)^3} \frac{d\xi_1 dx_1}{(2\pi)^3} \cdots \frac{d\xi_{n-1} dx_{n-1}}{(2\pi)^3} \\ & = \overbrace{\int_{\mathbf{R}^d} \cdots \int_{\mathbf{R}^d}}^{n \text{ times}} \prod_{l=1}^n \left\{ [e^{-i \frac{t}{n} \frac{1}{2}(-\Delta)}](x_l - x_{l-1}) e^{[A(\frac{x_l + x_{l-1}}{2}) \cdot (x_l - x_{l-1}) - \frac{t}{n} V(x_{l-1})]} \right\} g(x_0) \\ & \quad \times dx_0 dx_1 \cdots dx_{n-1}, \end{aligned}$$

where put $\xi_j = \Xi(t_j)$, $x_j = X(t_j)$, $j = 0, 1, \dots, n-1$, and $x = x_n = X(t_n) = X(t)$. This is what is meant by $G(t/n)^n g$.

Similarly, $e^{-t[-\frac{1}{2}(-i\nabla - A(x))^2 + V]}g$ should be given by the *imaginary-time phase space path integral* through time-sliced approximation as the $n \rightarrow \infty$ limit of the integral

$$\begin{aligned}
(4.12) \quad & \overbrace{\int_{\mathbf{R}^{2d}} \cdots \int_{\mathbf{R}^{2d}}}^{n \text{ times}} e^{\sum_{l=1}^n [i(X(t_l) - X(t_{l-1})) \cdot \Xi(t_{l-1}) - \frac{t}{n} \frac{1}{2} \Xi(t_{l-1})^2]} \\
& \times e^{\sum_{l=1}^n [iA\left(\frac{X(t_l) + X(t_{l-1})}{2}\right) \cdot (X(t_l) - X(t_{l-1})) - \frac{t}{n} V(X(t_{l-1}))]} g(X(0)) \prod_{j=1}^n \frac{d\Xi(t_{j-1}) dX(t_{j-1})}{(2\pi)^3} \\
& = \overbrace{\int_{\mathbf{R}^{2d}} \cdots \int_{\mathbf{R}^{2d}}}^{n \text{ times}} \prod_{j=1}^n \left\{ e^{[i(x_j - x_{j-1}) \cdot \xi_{j-1} - \frac{t}{n} \frac{1}{2} \xi_{j-1}^2]} e^{[iA\left(\frac{x_j + x_{j-1}}{2}\right) \cdot (x_j - x_{j-1}) - \frac{t}{n} V(x_{j-1})]} \right\} g(x_0) \\
& \quad \times \frac{d\xi_0 dx_0}{(2\pi)^3} \frac{d\xi_1 dx_1}{(2\pi)^3} \cdots \frac{d\xi_{n-1} dx_{n-1}}{(2\pi)^3} \\
& = \overbrace{\int_{\mathbf{R}^d} \cdots \int_{\mathbf{R}^d}}^{n \text{ times}} \prod_{j=1}^n \left\{ [e^{-\frac{t}{n} \frac{\Delta}{2}}](x_j - x_{j-1}) e^{[iA\left(\frac{x_j + x_{j-1}}{2}\right) \cdot (x_j - x_{j-1}) - \frac{t}{n} V(x_{j-1})]} \right\} g(x_0) \\
& \quad \times dx_0 dx_1 \cdots dx_{n-1},
\end{aligned}$$

where put $\xi_j = \Xi(t_j)$, $x_j = X(t_j)$, $j = 0, 1, \dots, n-1$, and $x = x_n = X(t_n) = X(t)$. This is what is meant by $G(t/n)^n g$. Equation (4.12) is suggesting us how that functional of the (Brownian) path $B(\cdot)$, which is to be created as the integrand of the Feynman–Kac–Itô formula (3.18) by the approximation $G(t/n)^n$, does look (See [S-05, (15.1-2), p.159]).

4.1.3. Dirac operator with vector and scalar potentials $A(x)$ and $V(x)$

The operator concerned is $\alpha \cdot (-i\nabla - A) + m\beta + V$ in $L^2(\mathbf{R}^3; \mathbf{C}^4)$ where $\alpha := (\alpha_1, \alpha_2, \alpha_3)$ and β are Dirac four matrices. Put

$$\begin{aligned}
(F(t)f)(x) &:= \int_{\mathbf{R}^3} K^{\text{Dirac}}(t, x - y) e^{i[A(\frac{x+y}{2})(x-y) - V(\frac{x+y}{2})t]} f(y) dy \\
(4.13) \quad &= \int_{\mathbf{R}^3} [e^{-it(\alpha \cdot (-i\nabla) + m\beta)}](x - y) e^{i[A(\frac{x+y}{2})(x-y) - V(\frac{x+y}{2})t]} f(y) dy
\end{aligned}$$

for $f \in L^2(\mathbf{R}^3; \mathbf{C}^4)$, where $K^{\text{Dirac}}(t, x - y) := [e^{-it(\alpha \cdot (-i\nabla) + m\beta)}](x - y)$ is the integral kernel of the unitary group of *free* Dirac operator $\alpha \cdot (-i\nabla) + m\beta$. Then, under certain reasonable conditions on $A(x)$ and $V(x)$, we have by Chernoff's theorem that as $n \rightarrow \infty$,

$$(4.14) \quad F(t/n)^n f \rightarrow e^{-it[(\alpha \cdot (-i\nabla - A) + m\beta) + V]} f, \quad \text{strongly.}$$

On the other hand, $e^{-it[\alpha \cdot (-i\nabla - A) + m\beta + V]} f$ should be given by the *phase space path integral* through time-sliced approximation as the $n \rightarrow \infty$ limit of the integral

$$\begin{aligned}
(4.15) \quad & \overbrace{\int_{\mathbf{R}^6} \cdots \int_{\mathbf{R}^6}}^{n \text{ times}} e^{i \sum_{l=1}^n [(X(t_l) - X(t_{l-1})) \cdot \Xi(t_{l-1}) - \frac{t}{n} (\alpha \cdot \Xi(t_{l-1}) + m\beta)]} \\
& \times e^{i \sum_{l=1}^n \left[A \left(\frac{X(t_l) + X(t_{l-1})}{2} \right) \cdot (X(t_l) - X(t_{l-1})) - \frac{t}{n} V(X(t_{l-1})) \right]} f(X(0)) \prod_{j=1}^n \frac{d\Xi(t_{j-1}) dX(t_{j-1})}{(2\pi)^3} \\
& = \overbrace{\int_{\mathbf{R}^6} \cdots \int_{\mathbf{R}^6}}^{n \text{ times}} \prod_{j=1}^n \left\{ e^{[i(x_j - x_{j-1}) \cdot \xi_{j-1} - i \frac{t}{n} (\alpha \cdot \xi_{j-1} + m\beta)]} e^{i \left[A \left(\frac{x_j + x_{j-1}}{2} \right) \cdot (x_j - x_{j-1}) - \frac{t}{n} V(x_{j-1}) \right]} \right\} \\
& \quad \times f(x_0) \frac{d\xi_0 dx_0}{(2\pi)^3} \frac{d\xi_1 dx_1}{(2\pi)^3} \cdots \frac{d\xi_{n-1} dx_{n-1}}{(2\pi)^3} \\
& = \overbrace{\int_{\mathbf{R}^3} \cdots \int_{\mathbf{R}^3}}^{n \text{ times}} \prod_{j=1}^n \left\{ [e^{-i \frac{t}{n} (\alpha \cdot (-\nabla) + m\beta)}] (x_j - x_{j-1}) [e^{i \left[A \left(\frac{x_j + x_{j-1}}{2} \right) \cdot (x_j - x_{j-1}) - \frac{t}{n} V(x_{j-1}) \right]} \right\} \\
& \quad \times f(x_0) dx_0 dx_1 \cdots dx_{n-1} \\
& = \overbrace{\int_{\mathbf{R}^3} \cdots \int_{\mathbf{R}^3}}^{n \text{ times}} K^{\text{Dirac}}\left(\frac{t}{n}, x_n - x_{n-1}\right) K^{\text{Dirac}}\left(\frac{t}{n}, x_{n-1} - x_{n-2}\right) \cdots K^{\text{Dirac}}\left(\frac{t}{n}, x_1 - x_0\right) \\
& \quad \times \left\{ e^{i \sum_{j=1}^n \left[A \left(\frac{x_j + x_{j-1}}{2} \right) \cdot (x_j - x_{j-1}) - \frac{t}{n} V(x_{j-1}) \right]} \right\} f(x_0) dx_0 dx_1 \cdots dx_{n-1}.
\end{aligned}$$

Here we have put $\xi_j = \Xi(t_j)$, $x_j = X(t_j)$, $j = 0, 1, \dots, n-1$, $x = x_n = X(t_n) = X(t)$, and in the last equality, we have performed all the $d\xi_j$ integrations. The last member of (4.15) is nothing but what is meant by $F(t/n)^n f$, and is suggesting us what a kind of functional of the path $X(\cdot)$ the expected path integral formula should turn out to have in its integrand. For instance, since $n \rightarrow \infty$,

$$\sum_{j=1}^n \left[A \left(\frac{x_j + x_{j-1}}{2} \right) \cdot (x_j - x_{j-1}) - \frac{t}{n} V(x_{j-1}) \right] \rightarrow \int_0^t [A(X(s)) \cdot dX(s) - V(X(s)) ds],$$

we should have an expression

$$\begin{aligned}
& \langle f_1, e^{-it[\alpha \cdot (-i\nabla - A) + m\beta + V]} f_2 \rangle \\
& = \int \int_{\mathbf{R}^3 \times \mathbf{R}^3} dx dy \langle f_2(x), d\nu_{t,x;0,y}^{\text{Dirac}}(X) e^{i \int_0^t [A(X(s)) \cdot dX(s) - V(X(s)) ds]} f_1(y) \rangle,
\end{aligned}$$

for all functions f_1, f_2 , say, in the Schwartz space $\mathcal{S}(\mathbf{R}^3; \mathbb{C}^4)$, if there should exist a 3×3 -matrix-valued (countable additive) measure $\nu_{t,x;0,y}^{\text{Dirac}}(X)$ on the space of Lipschitz-continuous paths $[0, t] \ni s \mapsto X(s) \in \mathbf{R}^3$ with $X(0) = y$, $X(t) = x$. However, no such measure $\nu_{t,x;0,y}^{\text{Dirac}}(X)$ can exist for this 3-dimensional Dirac operator $\alpha \cdot (-i\nabla - A) + m\beta + V$,

although it can for 1-dimensional Dirac operator instead (cf. [I-82, 84], [ITa-84, 87], [I-93]).

§ 4.2. Time-sliced approximation in norm and pointwise

4.2.1. Trotter–Kato product formula and Chernoff’s theorem in norm

In [IT-01, ITTZ-01], we proved the selfadjoint Trotter–Kato product formula *in norm*, i.e. *in operator norm*:

If A and B are nonnegative selfadjoint operators in a Hilbert space such that their operator sum $C := A + B$ is also selfadjoint with domain $D[C] := D[A] \cap D[B]$, then as $n \rightarrow \infty$, $(e^{-\frac{t}{n}A}e^{-\frac{t}{n}B})^n$ as well as $(e^{-\frac{t}{2n}B}e^{-\frac{t}{n}A}e^{-\frac{t}{2n}B})^n$ converges to e^{-tC} in operator norm, with optimal error estimate $O(n^{-1})$. This means nothing but that $F(t/n)^n \rightarrow e^{-tC}$ in operator norm, with $F(t) := e^{-tA}e^{-tB}$ or $F(t) := e^{-tB/2}e^{-tA}e^{-tB/2}$.

Applying this result to the Schrödinger semigroup with $H_V := -\frac{1}{2}\Delta + V$, where $V(x) \geq 0$ and H_V becomes a selfadjoint operator in $L^2(\mathbf{R}^d)$ with domain $D[H_V] = D[\Delta] \cap D[V]$, we have

$$\begin{aligned} (e^{-\frac{t}{n}\frac{1}{2}(-\Delta)}e^{-\frac{t}{n}V})^n &\rightarrow e^{-tH_V}, & \text{in operator norm,} \\ (e^{-\frac{t}{2n}V}e^{-\frac{t}{n}\frac{1}{2}(-\Delta)}e^{-\frac{t}{2n}V})^n &\rightarrow e^{-tH_V}, & \text{in operator norm,} \end{aligned}$$

as $n \rightarrow \infty$, with error estimate $O(n^{-1})$.

The proof of this operator-norm version of Trotter–Kato product formula is thanks to an operator-norm version of Chernoff’s theorem, even with error estimate, established also in [IT-01] (cf. [NeZ-99]). Only part of it without error estimate is given here.

Chernoff’s Theorem in operator norm. *Let $\{F(t)\}_{t \geq 0}$ be a family of selfadjoint operators in a Hilbert space with $0 \leq F(t) \leq 1$. Then if*

$$\|(1 + t^{-1}(I - F(t)))^{-1} - (1 + C)^{-1}\| \rightarrow 0, \quad t \downarrow 0,$$

with C some nonnegative selfadjoint operator, then

$$\|F(t/n)^n - e^{-tC}\| \rightarrow 0, \quad n \rightarrow \infty.$$

As for the *unitary Trotter product formula in operator norm*, it does not in general hold. For some counterexamples, see [I-03, pp.88–90]. However, there are some special cases where it holds for the unitary groups for the Dirac operator and the relativistic Schrödinger operator with *suitable potentials*. For the details, see [IT-04a].

4.2.2. Time-sliced approximation for Schrödinger equation in real and imaginary time — convergence in norm and pointwise

As touched on only briefly at the end of §4.2.1 just above, the unitary Trotter product formula in norm, i.e. in operator norm does not hold for the nonrelativistic Schrödinger operator $H_V = -\frac{1}{2}\Delta + V$ considered in §4.1.1.

However, we want to discuss a little more how about the convergence in operator norm and/or pointwise for the integral kernels by time-sliced approximation and to observe some remarkable fact on the error estimate of this approximation comparing the cases for the *real-time* and *imaginary-time* nonrelativistic Schrödinger equations.

First, for the *real-time* nonrelativistic Schrödinger equation $i\frac{\partial}{\partial t}\psi(t, x) = H_V\psi(t, x)$, we visit Fujiwara's result [Fu-79, 80], in particular, book [Fu-99, Theorems 4.22, 4.26, 5.4.1 (pp.79, 82, 105)] or survey [Fu-12, Theorems 3.3, 3.4 (p.105)], [FuKu-06, Theorem 2(p.843)] (cf. [Ku-04], [FuKu-05]). He made use of a sophisticated way of time-sliced approximation for Feynman path integral to construct the fundamental solution $e^{-itH_V}(x, y)$, i.e. the integral kernel of the Schrödinger unitary group e^{-itH_V} . It is a much more elaborate time-sliced approximation than the one naturally stemming from the Trotter product formula.

For explanation, let $V(x)$ be a smooth function satisfying $|\partial^\alpha V(x)| \leq C_\alpha(1 + x^2)^{(2-|\alpha|)_+/2}$ for every multi-index α with constant C_α , though $V(x)$ need not be bounded below. [For instance, this condition is satisfied by $V(x) = \pm|x|^2$.] Put

$$(4.16) \quad (E(t)\varphi)(x) = (2\pi it)^{-d/2} \int_{\mathbf{R}^d} e^{iS(t,x,y)} \varphi(y) dy$$

for $\varphi \in C_0^\infty(\mathbf{R}^d)$, with action $S(t, x, y) = \int_0^t [\frac{1}{2}(\frac{d\bar{X}(s)}{ds})^2 - V(\bar{X}(s))] ds$, where $\bar{X}(s)$ is the classical trajectory starting at $\bar{X}(0) = y$ and ending at $\bar{X}(t) = x$. Then Fujiwara proved, among others, that, for sufficiently small $t > 0$, the $n \rightarrow \infty$ limit of the integral kernel $[E(t/n)^n](x, y)$ of $E(t/n)^n$ exists pointwise and is equal to the integral kernel $e^{-itH_V}(x, y)$ of the Schrödinger unitary group e^{-itH_V} , i.e. the fundamental solution for the Schrödinger equation, and further that one has

$$(4.17) \quad [E(t/n)^n](x, y) - e^{-itH_V}(x, y) = O(n^{-1})t^2(2\pi t)^{-d/2},$$

as $n \rightarrow \infty$, uniformly in x, y , together with all the x, y -derivatives of the left-hand side, where $O(n^{-1})$ is independent of x, y and t . The proof also yields further that

$$(4.18) \quad \| [E(t/n)^n](x, y) - e^{-itH_V} \|_{L^2 \rightarrow L^2} = O(n^{-1}).$$

It turns out that this time-sliced approximation to the Schrödinger unitary group e^{-itH_V} converges both pointwise for the integral kernels and in operator norm, with error estimate $O(n^{-1})$.

Next, in the *imaginary-time* case, we will give a little more detailed account of the related situation than what was briefly mentioned in §4.2.1. Assume that $V(x)$ satisfies the condition that there exist constants $\rho \geq 0$ and $0 < \delta \leq 1$ such that $V(x) \geq C(1 + |x|^2)^{\rho/2}$ and $|\partial_x^\alpha V(x)| \leq C_\alpha(1 + |x|^2)^{(\rho - \delta|\alpha|)/2}$ for every multi-index α with constant C_α . Here the case $\delta = 0$ is allowed for $\rho = 0$. Therefore, in particular, it is the case if $V(x)$ is nonnegative and satisfies the same condition as Fujiwara's. Then the operator $H_V = -\frac{1}{2}\Delta + V$ becomes selfadjoint with domain $D[H_V] = D[-\frac{1}{2}\Delta] \cap [V]$. As noted in [I-03], so we can obtain analogous results for the Schrödinger semigroup e^{-tH_V} with the same error estimate $O(n^{-1})$ in operator norm by the general abstract theory in [IT-01, ITTZ-01] quoted in §4.2.1, and pointwise for the integral kernels as briefly sketched in [I-03, p.86].

However, we have in fact proved much more in [IT-04b, 06] that, with $F(t) := e^{-\frac{t}{2}V} e^{-t\frac{1}{2}(-\Delta)} e^{-\frac{t}{2}V}$, $F(t/n)^n$ converges to e^{-tH_V} with the error estimate $O(n^{-2})$, sharper than the general optimal $O(n^{-1})$, *both in operator norm and pointwise for the integral kernels*:

$$(4.19) \quad \|F(t/n)^n - e^{-tH_V}\|_{L^2 \rightarrow L^2} = O(n^{-2}),$$

$$(4.20) \quad [F(t/n)^n](x, y) - e^{-tH_V}(x, y) = O(n^{-2})t^2(2\pi t)^{-d/2}, \quad \text{uniformly on } \mathbf{R}^d \times \mathbf{R}^d,$$

locally uniformly in $t > 0$. The error estimate $O(n^{-2})$ here is also seen, in [AzI-08], to be optimal from below in [AzI-08]. Notice also that this error estimate $O(n^{-2})$ is sharper than in the real-time case (4.17), (4.18) of the nonrelativistic Schrödinger equation, though the two time-sliced approximations $E(t/n)^n$ and $F(t/n)^n$ are coming from quite different thoughts and ideas.

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